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From THE VACUUM LAB

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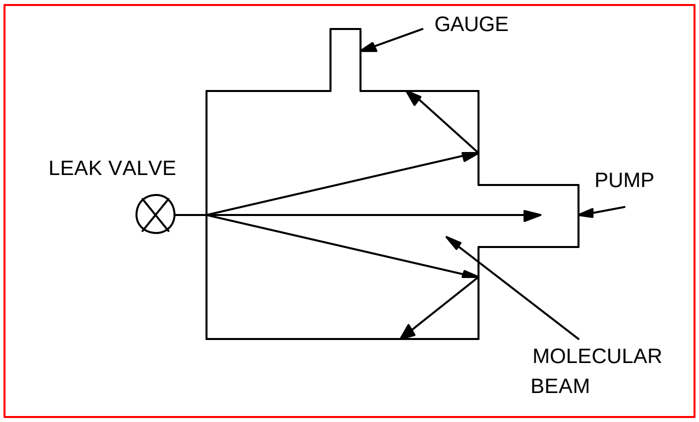
Solving Process Problems at the Molecular Flux Level

Working from pressure readings alone can mislead and misdirect a search for process problems, but reaching down a layer further into the molecular flux level can provide real solutions.

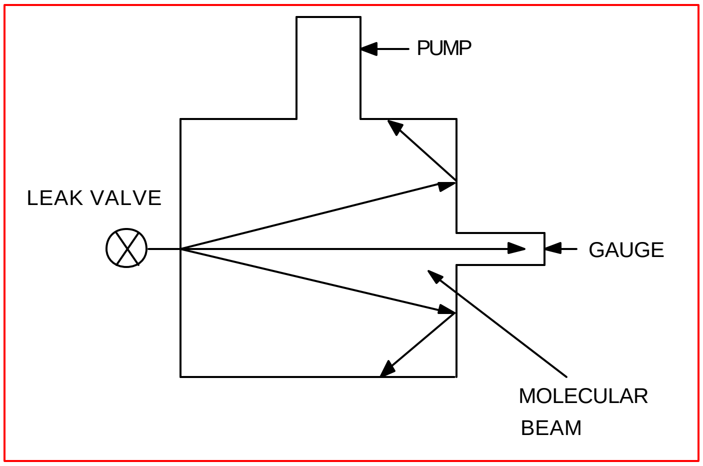
Every vacuum process has some sort of specified parameters that must be met if the process is to be either initiated or carried out successfully. Most commonly, these parameters specify that a certain vacuum level be achieved or maintained, and these levels are usually stated in either total pressure or in partial pressures of specific gases. Although parametric specificity at this level is often sufficient, there are all too many cases where process problems erupt even though the vacuum specs appear to be met or exceeded. This result, then, often causes the vacuum practitioner to question the original specifications even though they'd already proved to be apparently workable and practical. What's really missing in this situation is the awareness that all technologies, and vacuum in particular, exist in layers of detail and complexity. In this case, we can assume overdependence on the fundamental vacuum relationship; Q=SP.

The Q=SP relationship where Q is the gas load in torr Liters/sec., S is pumping speed in Liters/sec., and P is pressure in torr is an extremely important and essential tool to use for understanding the behavior of vacuum systems. It does, however, have a built-in trap that can interfere with a deeper understanding if we let it. We have to assume an equilibrium condition and a uniformity of gas load, pressure, and identity of gas species throughout a system to make use of it. When process or design problems require us to reach into a deeper level of understanding, it becomes apparent that the assumptions applied to the Q=SP relationship aren't necessarily true at this level. For example, the idea of a large number of gas molecules bouncing around within a chamber in purely random and mutually equidistant motion begins to break down. The Q=SP relationship is a bit of an abstraction that is useful for calculating and understanding overall performance, but it cannot take into account the actual detailed motion of molecules within the chamber. This level is where many problems are to be found. Specific sources of gas, often in the form of molecular beams, and specific gas sinks need to be considered and analyzed.

If we look at a commonly encountered problem such as a tiny pinhole leak, we can easily construct a mental picture of an expanding beam of molecules entering the chamber from the leak site. If we know the leak rate in common terms, such as torr Liters/sec., we can do a Q=SP calculation and determine the chamber pressure change engendered by the leak providing we know the pumping speed. If we know the change in chamber pressure, we can calculate the leak rate instead. A beam of non-polar air gases such as nitrogen (N_2) or oxygen (O_2) will enter an empty chamber, continually rebound from surfaces, reach an equilibrium concentration, and be pumped away. But, working at a lower level, we can see that the beam of chemically active gas could easily pass right through a work volume or could impact a work surface. This would have the same effect on the process as a total pressure many orders of magnitude higher. Process problems could then be encountered even though the pressure reading(s) was still within the approved process parameters. This is only a single example of the need to think in molecular flux instead of gas pressure.



The process gas enters the chamber, but most of it goes directly into the pump, and this provides a wrong pressure measurement.



The process gas enters the chamber, but most of it goes into the gauge, and this provides a wrong pressure measurement.

Thinking in molecular flux not only allows us to quantify the numbers of molecules acting and interacting within the system but also begins to allow us to build mental pictures of the performance of the system. Out of this ability to construct mental pictures will, in time and use, allow the vacuum practitioner to grow the priceless ability to “feel” a system perform. This painfully acquired skill can have many important practical applications in both troubleshooting a design or process and in the original system design or process development.

Units

In the Q=SP relationship, we make our calculations in units that are convenient for the abstract relationship but are difficult to think in. Gas loads (Q) in mass flow terns of torr Liters/sec. are very hard to picture mentally, but a stated number of molecules/sec. is much easier to handle effectively. After all, pressure is really the number of molecules in a given volume to anyone working in the molecular flow regime where the normal concept of pressure is essentially meaningless anyway. In many processes, the number of molecules passing through a process volume or impacting upon a process surface is key to understanding that process. Granted, the number of molecules/Liter/torr is a mindboggling number, but it does give us something to work with. This can be calculated with the following equation: (torr) x (3.54×10^{19}) = molecules/Liter. This kind of calculation can be useful when comparing the number of molecules in a volume and then adding in a particular beam-borne flux of molecules from something like a leak. It is even more useful to think (mental picture again) of the number of molecules impacting a surface. Assuming that all the residual molecules are N_2, we can calculate the number of collisions: (torr) x (3.95×10^{20}) = number of collisions/cm^2/sec. This an be compared to the number of collisions/sec. that would result from an impacting beam of molecules. The same system can be applied to the number of molecules passing through a process volume by merely calculating the surface area of the volume.

Practical Applications

Molecular flux concepts can be applied in either a qualitative or quantitative fashion. Qualitatively, we can use the surface impact calculations already discussed to determine the effects. For example, a freshly deposited film of active metal will react with the residual gases as they impact on the surface, so it becomes possible to make stoichiometric calculations of the chemical changes on the surface. That might well be to determine how long the fresh film can be exposed before an insulating film results. Before the quantitative calculations become important, though, we need to learn to think a system's possible performance through using molecular flux thinking techniques to determine whether there would be any effects additional to the obvious residual gas impacts.

We can then begin to think about, and mentally picture, what might occur when a process gas is introduced into a vacuum chamber. When a stream of gas is allowed to flow from a controlled leak valve into the chamber, it will tend to form an expanding molecular beam that traverses the chamber volume, and usually the process volume, in essentially a straight line. The beam's diameter will increase with distance and form a continuous cone with the molecular population greatest at the cone's center in a condition called cosine distribution. If a pump is located directly across the chamber from the leak valve, the greatest portion of the gas will be directed into the pump's throat with only the outlying portion of the beam striking the chamber wall. If the gauge sensor head is located 90^{o} from the line between valve and pump, it will only detect the gas that doesn't enter the pump as it scatters away from the chamber wall. This means that more gas is passing through the chamber and the process than would be expected from the gauge's pressure reading. If the gauge and pump positions are reversed, though, the gauge would detect a seemingly higher gas flux than would actually be the case. These two practical examples represent two common design mistakes that lead to process problems that aren't immediately apparent when the process is monitored by pressure readings alone.

Calculating Molecular Flux

Molecular Density

(3.54×10^{19}) x (torr) = Molecules/Liter

Molecule/Surface Collisions

(3.95×10^{20}) x (torr) = Collisions/cm^2/sec.

Mass Flow Rate (Throughput)

(3.54×10^{19}) x (torr Liters/sec.) = Molecules/sec.

(2.69×10^{19}) x (atm. cm^3/sec.) = Molecules/sec.

Molecular flux thinking allows us to take identified gas load sources and picture, or calculate, the effects of the resultant flux. For example, a large O-ring on a door seal can easily allow a diffusive flux from the O-ring's outgassing and permeation of water vapor. This can result in the build-up of sorbed water vapor on surfaces close to the O-ring that can later be a problem for a process if the surface desorption rate is too high. The number of examples and possible uses for this type of thinking and analysis is endless, but learning to use it on simple and fairly standard applications can help master the technique and make it a standard mental reflex when considering a design or trouble-shooting a system or process. The Q=SP relationship is a powerful tool and should never be ignored, but any vacuum practitioner should be constantly ready to peel back another layer in the technology and think molecular flux.

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